

SEARCH REQUEST FORM

7-540

Requestor's

Name:

Ted CRIARES

Serial

Number:

08/003208 ✓

Date:

9/29/83

Phone:

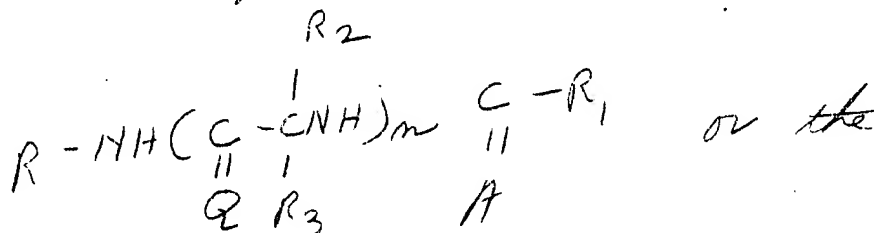
308-4607

Art Unit:

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).

Please search for the compound



N-oxide thereof

R and R₁ = anything

R₂ and R₃ = anything

A and Q are O or S but one must be S

see claim 1

FOR OFFICIAL USE ONLY

STAFF USE ONLY

Date completed:

7-50-43

Searcher:

JOHN DANT 7/1/83

Search Site

STIC

Vendors

IG Suite

=> fil reg

FILE 'REGISTRY' ENTERED AT 14:20:16 ON 30 SEP 93

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

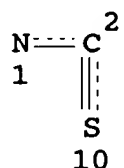
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STRUCTURE FILE UPDATES: 25 SEP 93 HIGHEST RN 150282-88-5

DICTIONARY FILE UPDATES: 28 SEP 93 HIGHEST RN 150282-88-5

=> d que 122

L3 STR



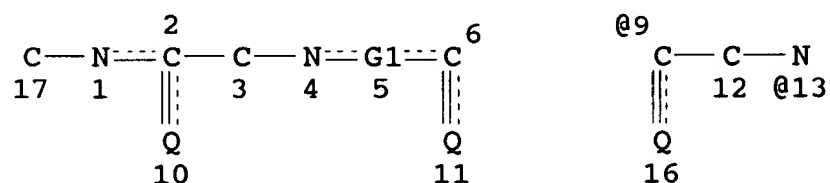
NODE ATTRIBUTES: NONE

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

L12 STR



REP G1=(0-3) 9-4 13-6

NODE ATTRIBUTES:

NSPEC IS RC AT 17

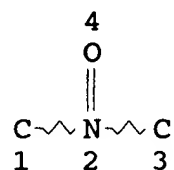
CONNECT IS M2 RC AT 1

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

L18 STR



NODE ATTRIBUTES:

CONNECT IS E1 RC AT 4

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 4

L21 1485 SEA FILE=REGISTRY SSS FUL L12 AND L3

L22 1 SEA FILE=REGISTRY SUB=L21 SSS FUL L18

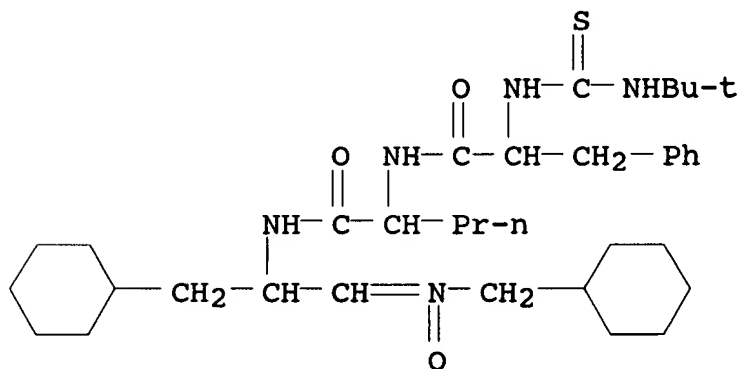
=> d 122 all

N-oxide

L22 ANSWER 1 OF 1 COPYRIGHT 1993 ACS
 RN 131806-79-6 REGISTRY
 CN Norvalinamide, N-[[[(1,1-dimethylethyl)amino]thioxomethyl]-L-phenylalanyl-N-[2-cyclohexyl-1-[[[(cyclohexylmethyl)imino]methyl]ethyl]-, N-oxide, (S)- (9CI) (CA INDEX NAME)
 MF C35 H57 N5 O3 S
 SR CA
 LC CA
 DES *

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.1	2
C6	C6	6	C6	46.150.18	1



N-oxide
★

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1

AN CA114(9):82554t
 TI Preparation of [(peptidylamino)propylidene]amine N-oxides as inhibitors for renin and retroviral proteinases
 AU Rueger, Wolfgang; Urbach, Hansjoerg; Ruppert, Dieter; Schoelkens, Bernward
 CS Hoechst A.-G.
 LO Fed. Rep. Ger.
 SO Ger. Offen., 17 pp.
 PI DE 3842067 A1 21 Jun 1990
 AI DE 88-3842067 14 Dec 1988
 IC ICM C07K005-06
 ICS C07K005-08; C07K001-06; C07K001-08; C07K001-10; A61K037-02; A61K031-195
 SC 34-3 (Amino Acids, Peptides, and Proteins)
 SX 1
 DT P
 CO GWXXBX

PY 1990
 LA Ger
 AB R1-A-D-CHR3CO-B-NHCHR2CH:N(O)R4 [I; R1 = H, (un)substituted C1-18 alkyl, C3-7 cycloalkyl, C6-14 aryl, 5-7 membered (un)substituted heterocyclyl, etc.; R2 = H, C1-10 alkyl, C4-7 cycloalkyl, C6-14 aryl, 4-7 membered O- or S-contg. heterocyclyl; R3 = (un)substituted C6-14 aryl, C6-14 aryl(C1-14 alkyl), (un)substituted thienyl or pyridyl; R4 = (un)substituted C1-8 alkyl, C3-8 cycloalkyl, C6-14 aryl, etc.; A = bond, S, O, etc.; B = amino acid residue], and their physiol. compatible salts, are prepd. I are useful as antihypertensives and for the treatment of heart insufficiency and viral diseases (no data). Thus, N-[3-cyclohexyl-(2S)-(N-tert-butoxycarbonyl-L-phenylalanyl-L-histidylamino)propylidene]-N-[(1S)-ethoxycarbonyl-2-methyl-2-propyl]amine N-oxide was prepd. by soln.-phase coupling of BOC-Phe-His(DNP)-OH (DNP = 2,4-dinitrophenyl) with N-[(2S)-amino-3-cyclohexylpropylidene]-N-[(1S)-ethoxycarbonyl-2-methyl-1-propyl]amine N-oxide (prepn. of both compds. given). I in vitro inhibited renin with IC50 of 10-5 to 10-10 M and HIV-proteinase with IC50 of 10-4 to 10-8M.

KW peptidylaminopropylideneamine oxide prepn renin inhibitor; amine oxide peptidylaminopropylidene renin inhibitor; HIV proteinase inhibitor peptide prepn; antihypertensive peptide amide prepn; heart insufficiency treatment peptide prepn; antiviral peptide prepn

IT Peptides, preparation
 ((peptidylaminopropylidene)amine oxides, prepn. of, as renin and retroviral proteinase inhibitors)

IT 9015-94-5, Renin, biological studies
 (inhibitors, (peptidylaminopropylidene)amine oxides as)

IT 9001-92-7, Proteinase
 (of HIV, inhibition of, by (peptidylaminopropylidene)amine oxides)

IT 115766-13-7P
 (prepn. and reaction of, in prepn. of renin and retroviral proteinase inhibitor)

IT 3217-92-3P 4715-11-1P 78746-56-2P 98105-42-1P 110695-91-5P
 130129-73-6P 130129-74-7P 130129-75-8P 131806-52-5P
 131806-53-6P 131806-54-7P 131806-55-8P 131806-56-9P
 131806-57-0P 131806-58-1P 131806-59-2P 131806-60-5P
 131806-61-6P 131806-62-7P
 (prepn. of, as intermediate for renin and retroviral proteinase inhibitor peptides)

IT 131806-71-8P 131806-72-9P 131806-73-0P 131806-74-1P
 131806-75-2P 131806-76-3P 131806-77-4P 131806-78-5P
 131806-79-6P 131806-80-9P 131806-81-0P 131806-82-1P
 131806-83-2P 131899-03-1P 131899-04-2P 131899-05-3P
 131899-06-4P
 (prepn. of, as renin and retroviral proteinase inhibitor)

IT 109-90-0, Ethyl isocyanate 123-11-5, 4-Methoxybenzaldehyde, reactions 593-77-1, N-Methylhydroxylamine 1117-97-1 2043-61-0, Cyclohexanecarbaldehyde 3674-06-4 5042-80-8 17609-47-1 25024-53-7 37736-82-6 50632-53-6, N-Isopropylhydroxylamine hydrochloride 56558-30-6 123706-59-2 131806-84-3
 (reaction of, in prepn. of renin and retroviral proteinase inhibitor)

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=> d his

(FILE 'HOME' ENTERED AT 13:41:12 ON 30 SEP 93)
SET PAGELENGTH SCROLL
SET COST OFF

FILE 'REGISTRY' ENTERED AT 13:41:23 ON 30 SEP 93

L1 STR
L2 50 S L1
L3 STR L1
L4 50 S L1 AND L3
L5 STR L1
L6 50 S L5
L7 102 S L6 OR L4 OR L2
L8 0 S OXIDE AND L7
L9 STR L3
L10 STR L3
L11 50 S L5 AND L10
L12 STR L5
L13 50 S L12 AND L10
L14 STR
L15 15 S L12 AND L14
L16 2 S L15 AND OXIDE
L17 0 S L12 AND L3 AND L14
L18 STR L14
L19 0 S L12 AND L3 AND L18
L20 50 S L12 AND L3
L21 1485 S L12 AND L3 FUL
L22 1 SEARC L18 SUB=L21 FUL

1485 cmpds

FILE 'REGISTRY' ENTERED AT 14:20:16 ON 30 SEP 93

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=> fil ca

FILE 'CA' ENTERED AT 14:21:29 ON 30 SEP 93

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FILE COVERS 1967 - 18 Sept 93 (930918/ED) VOL 119 ISS 12.

=> s 121

L23 432 L21

— 432 citations

=> s 123 and us/pc

228705 US/PC

L24 26 L23 AND US/PC

← 26 US patents

=> d bib abs hitn

L24 ANSWER 1 OF 26 COPYRIGHT 1993 ACS

AN CA118(11):102481e

TI Preparation of N-(bisalkoxyphosphoryl)peptides as renin inhibitors

AU Doherty, Annette M.; Hamilton, Harriet W.; Steinbaugh, Bruce A.

CS Warner-Lambert Co.

LO USA

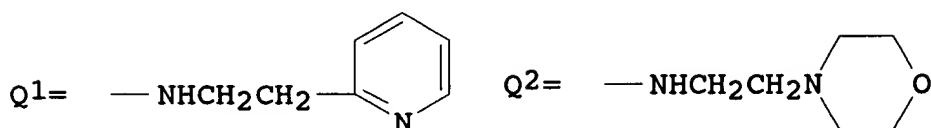
SO U.S., 26 pp.

PI US 5149692 A 22 Sep 1992

AI US 89-454795 21 Dec 1989

IC ICM C07K005-06

ICS C07K005-08
 NCL 514018000
 SC 34-3 (Amino Acids, Peptides, and Proteins)
 SX 1
 DT P
 CO USXXAM
 PY 1992
 LA Eng
 OS MARPAT 118:102481
 AN CA118(11):102481e
 GI



AB AXYWU [I; A = R1O(RO)P(O); R, R1 = H, PhCH2, alkyl, alkenyl; X = Phe, Tyr, Tyr(OMe), homophenylalanyl, cyclohexylalanyl, Leu, Trp, His, MePhe; Y = Gln, His, Leu, Met, Met(O), Met(O2), 2S-aminopentanoyl, 2S-amino-3-(4-thiazolyl)propanoyl, 2S-amino-4-pentenoyl, etc.; W = statinyl, 4S-amino-3S-hydroxy-5-cyclohexanepentanoyl, 3RS,4S-diamino-6-methylheptanoyl, etc.; U = H, NHCH2CH2N(CH2CH2OH)2, morpholino, Q2, Q2], were prepd. Thus, BOC-Alg-Cysta-Aen [Alg = 2S-amino-4-pentenoyl, Cysta = 4S-amino-3S-hydroxy-5-cyclohexanepentanoyl, Aen = N-(2-aminoethyl)morpholine] was stirred with CF3CO2H in CH2Cl2 and the residue was treated with HCl in CH2Cl2. The product was stirred with (Me2CH)2NEt, Q3-Phe-OH [Q3 = (Me2CH)2P(O)] (prepn. given), hydroxybenzotirazole, and DCC in DMF to give Q3-Phe-Alg-Cysta-Aen. The latter inhibited renin with IC50 = 0.97 .times. 10-9 M.

IT 61172-71-2P 90600-20-7P 110497-19-3P 118233-28-6P
 118272-81-4P 118317-76-3P 119808-16-1P 119808-65-0P
 119808-68-3P 124278-65-5P 135704-31-3P 145705-36-8P
 145705-37-9P 145705-38-0P 145705-39-1P 145705-40-4P
 145705-41-5P 145705-42-6P 145705-43-7P 145705-52-8P
 145774-98-7P 145774-99-8P 145775-00-4P 145775-01-5P
 145841-09-4P
 (prepn. of, as intermediate for renin inhibitor)

=> d bib abs hitrn 2-10

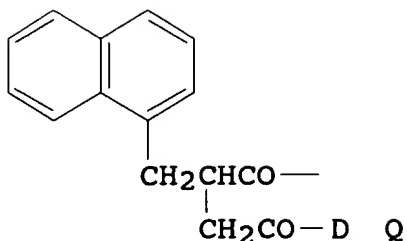
L24 ANSWER 2 OF 26 COPYRIGHT 1993 ACS
 AN CA118(3):22635t
 TI Peptide derivatives of 3-amino-2-hydroxypropionic acid as inhibitors of renin
 AU Hamilton, Harriet W.; Patt, William C.
 CS Warner-Lambert Co.
 LO USA
 SO U.S., 14 pp.
 PI US 5135914 A 4 Aug 1992
 AI US 88-197547 23 May 1988
 IC ICM A61K031-415
 ICS C07D233-64

NCL 514019000
SC 34-3 (Amino Acids, Peptides, and Proteins)
SX 1
DT P
CO USXXAM
PY 1992
LA Eng
OS MARPAT 118:22635
AN CA118(3):22635t
AB R1CH2CHR2CONHCHR3CONHCHR4CH(OH)COR5 [R1 = naphthyl
(substituted)phenyl, alkoxy; R2 = morpholinocarbonylmethyl,
naphthylmethyl, Me3CO2CNH, PhCOCH2, aminosulfonylamino; R3 =
4-imidazolyl, alkoxy, carbonyl, substituted aminoalkyl; R4 =
cyclohexylmethyl, Me2CHCH2; R5 = alkoxy, alkylamino, phenylalkyl,
pyridinylalkyl, heterocyclyl; provisos given], were prepd. Thus,
.alpha.-(1-naphthylmethyl)-1-naphthalenepropanoic acid was coupled
with iso-Pr [2R-[2R*, 3S*(S*)]]-3-[[2-amino-1-oxo-3-[1-
(triphenylmethyl)-1H-imidazol-4-yl]propyl]amino]-2-hydroxy-5-
methylhexanoate using DCC/1-hydroxybenzotriazole in DMF and the
product was heated in HOAc at 100.degree. to give iso-Pr [2R-[2R*,
3S*(S*)]]-2-hydroxy-3-[[3-(1H-imidazol-4-yl)-2-[[3-(1-naphthalenyl)-
2-(1-naphthalenylmethyl)-1-oxopropyl]amino]-1-oxopropyl]amino]-5-
methylhexanoate. The latter inhibited resin with IC50 = 1.4 .times.
10-7 M.

IT 144980-10-9P 144980-11-0P 144980-12-1P 144980-13-2P
144980-14-3P 144980-15-4P 145033-10-9P
145033-11-0P 145107-12-6P
(prepn. of, as renin inhibitor)

L24 ANSWER 3 OF 26 COPYRIGHT 1993 ACS
AN CA116(9):84192p
TI Preparation of peptides as renin inhibitors for treatment of
hypertension
AU Doherty, Annette M.; Hudspeth, James P.; Kaltenbronn, James S.;
Repine, Joseph T.; Roark, William H.; Sircar, Ila; Tinney, Francis
J.
CS Warner-Lambert Co.
LO USA
SO U.S., 88 pp. Cont.-in-part of U.S. Ser. No. 113,278, abandoned.
PI US 5024994 A 18 Jun 1991
AI US 88-233320 17 Aug 1988
PRAI US 86-945582 23 Dec 1986
US 87-113278 2 Nov 1987
IC ICM A61K037-02
ICS C07K005-00

NCL 514018000
SC 34-3 (Amino Acids, Peptides, and Proteins)
SX 1
DT P
CO USXXAM
PY 1991
LA Eng
OS MARPAT 116:84192
AN CA116(9):84192p
GI



AB Acyl-X-Y-W-U-V [acyl = BOC, isovaleryl, n-valeryl, Q, DNMA, etc.; DNMA = di(1-naphthylmethyl)acetyl; D = MeO, heterocyclyl, NMeCH₂CO₂Me; X = Phe, homophenylalanine residue, cyclohexylalanine residue, etc.; Y = .alpha., .omega.-diamino acid residue; W = STA, 4(S)-amino-3(S)-hydroxy-5-phenylpentanoic acid residue, 4(S)-amino-3(S)-hydroxy-5-cyclohexanepentanoic acid residue; STA = 4(S)-amino-3(S)-hydroxy-6-methylheptanoic acid residue; U = Leu, Ile, Val, MeLeu, MeIle; V = substituted amino] and their pharmaceutically acceptable salts were prepd. ClCH₂C.tplbond.CCH₂NHAc (prepn. given) was condensed with DNMA-NHCH(CO₂Et)₂ [prepd. from DNMA-Cl and H₂NCH(CO₂Et)₂] and the resulting DNMA-NHC(CHO₂Et)₂CH₂C.tplbond.CCH₂NHAc decarboxylated and then hydrolyzed to give DNMA-NHCH(CO₂H)CH₂C.tplbond.CCH₂NHAc, which was coupled with H-STA-NHCH₂CHMeEt to give two diastereomers of DNMA-NHCH[CH₂C.tplbond.CCH₂NHAc]CO-STA-NHCH₂CHMeEt. The diastereomer that was more sol. in EtOAc had an IC₅₀ of 2.9 .times. 10⁻⁸M against the activity of renin in vitro.

IT	1069-48-3P	3054-07-7P	14109-62-7P	14328-63-3P	17461-58-4P
	25543-13-9P	29052-82-2P	42998-51-6P	61016-49-7P	61172-71-2P
	75937-26-7P	77369-60-9P	97920-08-6P	100002-50-4P	
	100002-57-1P	100002-81-1P	104597-05-9P	110696-07-6P	
	115198-71-5P	115226-22-7P	118272-80-3P	118272-81-4P	
	118283-25-3P	118304-86-2P	118317-76-3P	118374-54-2P	
	119808-00-3P	119808-03-6P	119808-05-8P	119808-09-2P	
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	119808-15-0P	119808-16-1P	119808-17-2P	119808-18-3P	
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	119808-85-4P	119808-86-5P	119808-87-6P	119808-88-7P	
	119832-12-1P	119857-52-2P	124278-62-2P	124278-64-4P	
	124278-65-5P	132101-67-8P	132101-95-2P	132101-96-3P	
	138643-19-3P	138643-20-6P	138643-21-7P	138643-22-8P	
	138643-23-9P	138643-24-0P	138643-25-1P	138643-26-2P	
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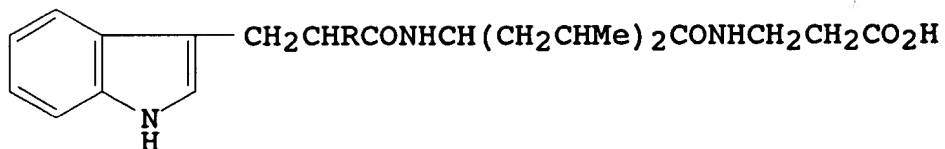
(prepn. of, as intermediate for renin-inhibiting peptides)

IT	26061-11-0P	119808-02-5P	119808-04-7P	119808-14-9P
	119808-67-2P	119808-72-9P	119808-73-0P	119808-74-1P
	119808-75-2P	119808-76-3P	119808-77-4P	119808-78-5P
	119808-79-6P	119808-80-9P	119808-93-4P	
	119808-94-5P	119808-95-6P	119808-97-8P	
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	119809-25-5P	119809-27-7P	119832-13-2P	119832-14-3P
	119906-26-2P	132101-72-5P	132101-73-6P	132101-74-7P
	132101-75-8P	132101-78-1P	132101-79-2P	
	132101-80-5P	132101-85-0P	132101-86-1P	132101-87-2P
	132199-76-9P	138643-06-8P	138643-07-9P	138643-08-0P
	138643-09-1P	138643-10-4P	138643-11-5P	138643-12-6P
	138643-13-7P	138643-14-8P	138643-15-9P	
	138643-16-0P	138643-17-1P	138643-18-2P	
	138677-39-1P	138677-40-4P	138677-41-5P	138750-37-5P
	138750-38-6P	138750-39-7P	138750-40-0P	138750-41-1P
	138750-42-2P	138750-43-3P	138750-44-4P	
	138750-45-5P			

(prepn. of, as renin inhibitor)

L24 ANSWER 4 OF 26 COPYRIGHT 1993 ACS
 AN CA115(13):136789q
 TI Preparation of C-terminal gastrin antagonists
 AU Murphy, Richard Finbar; Douglas, Alistair J.; Walker, Brian
 LO USA
 SO U.S., 35 pp.
 PI US 4997950 A 5 Mar 1991
 AI US 89-341084 20 Apr 1989
 IC ICM C07D473-00
 ICS C07D209-20
 NCL 548303000
 SC 34-3 (Amino Acids, Peptides, and Proteins)
 SX 1
 DT P
 CO USXXAM
 PY 1991
 LA Eng
 OS MARPAT 115:136789
 AN CA115(13):136789q

GI



I

AB Title compds. I (R = biotin-NH, dansyl-NH, fluorescein-NH, H, NH₂), antagonists of gastrin-stimulated acid secretion, are prepd. I were used to study structural activity of mol. and also to det. the smallest and highest affinity inhibitor of gastrin. Even small di- and tripeptide derivs. of gastrin C-terminal fragment with varied resistance to hydrolysis can exhibit antagonist activity to pentagastrin simulated gastric secretion. BOC-Leu-.beta.-Ala benzyl ester (prepn. given) was deprotected for 1 h in HCl/Et₂O, indole-3-propionic acid was coupled to the deprotected dipeptide ester to give the benzyl ester, which was removed by catalytic transfer hydrogenolysis to give I (R = H) (II) which was pptd. as the dicyclohexylamine salt. II showed 62.5% inhibition of pepsin secretion from gastric fistula.

IT 52716-48-0P 73545-96-7P 129505-35-7P 129505-36-8P
129524-77-2P **135892-75-0P** 135892-76-1P 135892-78-3P

(prepn. and deprotection of)

IT 3303-84-2P 53363-89-6P 54518-92-2P 68172-12-3P 87421-27-0P
99701-61-8P 109522-19-2P 109522-21-6P 135892-64-7P
135892-69-2P 135892-70-5P 135892-71-6P 135892-72-7P
135892-73-8P 135892-74-9P 135892-79-4P 135892-80-7P
135892-81-8P

(prepn. and peptide coupling of, in prepn. of gastrin antagonist peptide)

IT **109522-13-6P 109522-14-7P 109522-15-8P**
116339-46-9P 116652-97-2P 122855-47-4P 127745-41-9P
129505-37-9P 129505-38-0P 129505-40-4P 129505-42-6P
129505-44-8P 135892-53-4P 135892-54-5P **135892-55-6P**
135892-56-7P 135892-57-8P 135892-58-9P 135892-59-0P
135892-60-3P 135892-61-4P 135892-62-5P **135970-00-2P**
135970-01-3P

(prepn. of, as gastric secretion inhibitor)

L24 ANSWER 5 OF 26 COPYRIGHT 1993 ACS

AN CA114(7):61705c

TI Preparation of 2-(disubstituted amino)acetanilide herbicides

AU Wee, Siok Hui H.

CS ICI Americas, Inc.

LO USA

SO U.S., 13 pp.

PI US 4944796 A 31 Jul 1990

AI US 88-270573 14 Nov 1988

IC ICM A01N037-26

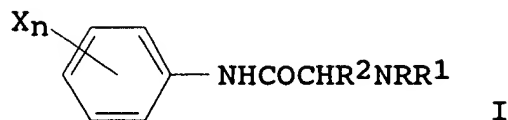
ICS C07C103-64; C07C103-82

NCL 071118000

SC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

SX 5

DT P
 CO USXXAM
 PY 1990
 LA Eng
 OS MARPAT 114:61705
 AN CA114(7):61705c
 GI



AB Title compds. I (R = alkyl, Ph; R1 = amino, alkyl, allyl, substituted carbonyl or carbamyl, alkythiothiocarbonyl, mono-haloanilinocarbonylmethylene, alkoxycarbonylmethylene, carboxymethylene; R2 = H, alkyl, Ph; X = halo, haloalkyl; n = 1-3) are prepd. To a CH2Cl2 soln. of 2,5-difluorosarcosineanilide and pyridine was added (F3CCO)2O and the mixt. was stirred for 2 h at room temp. to give I (R = Me; R1 = F3CCO; R2 = H; Xn = 2,5-F2). I (R = Me; R1 = EtSCO; R2 = H; Xn = 2,5-F2) at 4.48 kg/ha pre- and postemergence gave 100% control of Brassica kaber, Abutilon theophrasti, Ipomoea purpurea, and av. broadleaf.

IT	131654-85-8P	131654-86-9P	131654-87-0P	131654-88-1P
	131654-89-2P	131654-90-5P	131654-91-6P	131654-92-7P
	131654-93-8P	131654-94-9P	131654-95-0P	131654-96-1P
	131654-97-2P	131654-98-3P	131654-99-4P	131655-00-0P
	131655-01-1P	131655-02-2P	131655-03-3P	131655-04-4P
	131655-05-5P	131655-06-6P	131655-07-7P	131655-08-8P
	131655-09-9P	131655-10-2P	131655-11-3P	131655-12-4P
	131655-13-5P	131655-14-6P	131655-15-7P	131655-16-8P
	131655-17-9P	131655-18-0P	131655-19-1P	131655-20-4P
	131655-21-5P	131655-22-6P	131655-23-7P	131655-24-8P
	131655-25-9P	131655-26-0P	131655-27-1P	131655-28-2P
	131655-29-3P	131671-72-2P	131671-73-3P	131671-74-4P
	131671-75-5P			

(prepn. of, as herbicide)

L24 ANSWER 6 OF 26 COPYRIGHT 1993 ACS

AN CA112(23):217467y

TI Preparation of 2'- or 5'-aminodeoxynucleoside phosphoramidites and their use for the preparation of oligonucleotides having aliphatic amino groups

AU Smith, Lloyd M.; Fung, Steven

CS California Institute of Technology

LO USA

SO U.S., 30 pp. Cont.-in-part of U.S. Ser. No. 565,010, abandoned.

PI US 4849513 A 18 Jul 1989

AI US 86-878045 24 Jun 1986

PRAI US 83-565010 20 Dec 1983

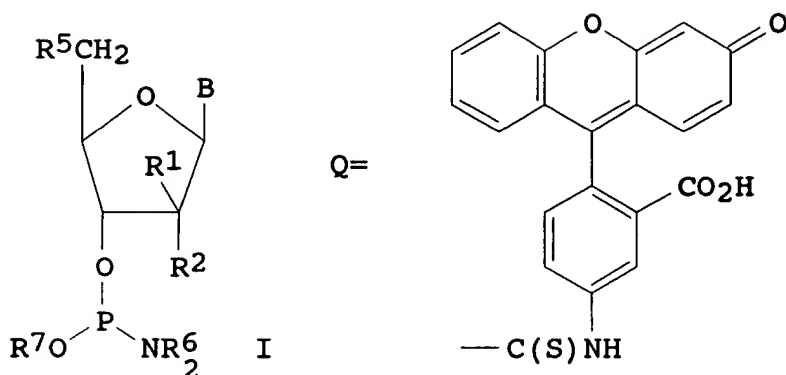
US 85-709579 8 Mar 1985

IC ICM C07H019-10

ICS C07H019-20

NCL 536027000

SC 33-9 (Carbohydrates)
 SX 9
 DT P
 CO USXXAM
 PY 1989
 LA Eng
 OS MARPAT 112:217467
 AN CA112(23):217467y
 GI



AB The title compds. [I; B = adenin-9-yl, guanin-9-yl, thymin-1-yl, cytosin-1-yl, uracil-1-yl, inosin-9-yl; R¹, R², R⁵ = H, OR, NHR⁸, with the proviso that one of R², R², and R⁵ = NHR⁸, and only R⁵ can be OH; R = monovalent C1-25 organ. protecting group; R⁸ = N-protecting group; R⁶ = lower alkyl, heterocycllyl; R⁷ = lower (cyano, halo, or nitrophenyl)alkyl], useful for the solid phase synthesis of oligonucleotide having aliph. NH₂ groups which can be covalently linked to fluorescent dyes or other detectable moieties to give the corresponding labeled oligonucleotides, e.g. as DNA hybridization probes, are prepd. Thus, N-acylation of 5'-amino-5'-deoxythymidine by 9-fluorenylmethyl chloroformate in DMF contg. (isoPr)₂NEt gave 5'-N-(9-fluorenylmethyloxycarbonyl)-5'-amino-5'-deoxythymidine which was treated 60 min with (isoPr)₂NPClOMe in the presence of (isoPr)₂NEt in CH₂Cl₂ to give I (B = thymin-1-yl, R¹ = R² = H, R⁵ = (9-fluorenylmethyloxycarbonyl)amino, R⁶ = isoPr, R⁷ = Me) (II). An oligodeoxyribonucleotide 3'-HOCpApTpGpCpTpCpT-NH₂-5' (III) was prepd. by the solid phase method using II. Reaction of III with fluorescein-5-isothiocyanate in 1M aq. NaHCO₃-Na₂CO₃ buffer (pH9) gave 3'-HOCpApTpGpCpTpCpT-NHQ-5'. Conjugation of eosin-5-isothiocyanate and Texas Red with 3'-HO(Tp)₆T-MH₂-5' on a solid support gave the corresponding fluorescent dye-labeled oligonucleotides.

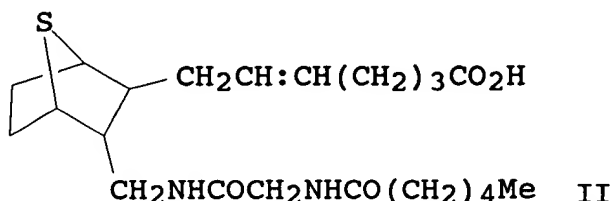
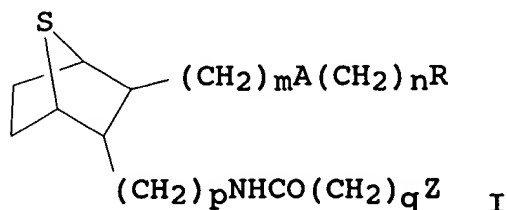
IT 118849-40-4P 126160-68-7P
 (prepn. of, for nucleic acid hybridization)

L24 ANSWER 7 OF 26 COPYRIGHT 1993 ACS
 AN CA112(19):172344n
 TI Irreversible inhibitors of adenosine receptors
 AU Jacobson, K. A.

CS United States Dept. of Health and Human Services
LO USA
SO U. S. Pat. Appl., 31 pp. Avail. NTIS Order No. PAT-APPL-7-221 413.
PI US 221413 A0 1 Jul 1989
AI US 88-221413 19 Jul 1988
SC 1-11 (Pharmacology)
SX 28
DT P
CO XAXXAV
PY 1989
LA Eng
AN CA112(19):172344n
AB Irreversible ligands for adenosine receptors based on
8-aryl-substituted xanthines as antagonists or N6-substituted
adenosines as agonists are prepd. as pharmaceuticals. Functionalized
congeners are provided which contain electrophilic acylating and
alkylating groups for reaction at nucleophilic residues of adenosine
receptors. Improved diuretics, kidney-protective agents, cardiotonic
agents, immunostimulants, vasodilators, antidiuretics, and
immunosuppressants are described.

IT 96760-69-9P 96865-89-3P 96865-92-8P 100892-75-9P
100892-77-1P 104344-31-2P 117723-91-8P 117723-92-9P
117723-93-0P 117723-96-3P 120059-09-8P 120059-11-2P
120059-13-4P 120059-16-7P 120059-17-8P 120059-18-9P
120059-19-0P 120059-20-3P 120059-21-4P 120059-22-5P
120059-23-6P 120059-25-8P 120059-26-9P 120059-28-1P
120059-31-6P 120059-33-8P 120059-34-9P 120059-36-1P
120059-37-2P 120059-38-3P 120059-39-4P 120059-40-7P
120059-42-9P 120085-28-1P 120085-29-2P 120085-30-5P
120085-31-6P 126433-03-2P 126433-04-3P 126463-01-2P
(prepn. of and adenosine receptor inhibition by)

L24 ANSWER 8 OF 26 COPYRIGHT 1993 ACS
AN CA110(13):114554d
TI Preparation of [(amidoalkyl)thiabicycloheptanyl]alkan- and -enoates
as platelet aggregation and bronchoconstriction inhibitors
AU Nakane, Masami
CS Squibb, E. R., and Sons, Inc.
LO USA
SO U.S., 44 pp.
PI US 4735962 A 5 Apr 1988
AI US 86-916083 6 Oct 1986
IC ICM C07D409-06
ICS C07D333-78; @@@@@@@-@@@
NCL 514382000
SC 26-3 (Biomolecules and Their Synthetic Analogs)
SX 1
DT P
CO USXXAM
PY 1988
LA Eng
OS MARPAT 110:114554
AN CA110(13):114554d
GI



AB The title compds. [I; A = CH₂CH₂, CH:CH; R = CO₂H, alkoxycarbonyl, alkali metal carboxylate, polyhydroxyalkylammonium carboxylate, (5-tetrazolyl)hydroxymethyl, CONR₃R₄; R₃, R₄ = H, alkyl, OH, alkoxy, aryl; Z = NR₁COR₂, NR₁CSR₂, CONR₁R₂, CSNR₁R₂, R₂NHCO₂; R₁ = H, alkyl; R₂ = R₁, alkenyl, alkynyl, etc.; m, p = 1-4; n = 1-5; q = 1-12] were prep'd. as platelet aggregation and bronchoconstriction inhibitors (no data). Title compd. II was prep'd. in 20 steps starting with AcOCH:CHCH:CH₂ and p-quinone.

IT	117232-66-3P	117232-67-4P	117232-68-5P	117232-69-6P
	117232-70-9P	117232-71-0P	117232-72-1P	117232-73-2P
	117232-74-3P	117232-75-4P	117232-76-5P	117232-77-6P
	117232-78-7P	117232-79-8P	117232-80-1P	117232-81-2P
	117232-82-3P	117232-83-4P	117232-84-5P	117232-85-6P
	117232-86-7P	117232-87-8P	117232-88-9P	117232-89-0P
	117232-90-3P	117232-91-4P	117232-92-5P	117232-93-6P
	117232-94-7P	117232-95-8P	117232-96-9P	117232-97-0P
	117232-98-1P	117232-99-2P	117233-00-8P	117233-01-9P
	117233-02-0P	117233-05-3P	117233-06-4P	117233-07-5P
	117404-56-5P			

(prepn. of, as platelet aggregation and bronchoconstriction inhibitor)

L24 ANSWER 9 OF 26 COPYRIGHT 1993 ACS

AN CA110(7):58104t

TI Preparation and testing of peptide thioneamides as selective substrates for cysteine proteases

AU Cho, Kyujin; Rasnick, David W.

CS Enzyme Systems Products, Inc.

LO USA

SO U.S., 6 pp.

PI US 4771123 A 13 Sep 1988

AI US 86-838531 11 Mar 1986

IC ICM C07K005-02

ICS C07K007-02

NCL 530323000

SC 34-3 (Amino Acids, Peptides, and Proteins)

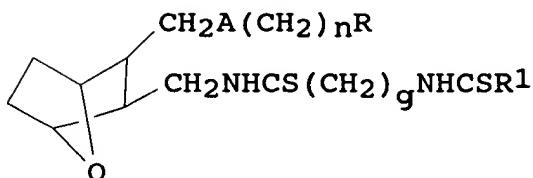
SX 1, 9

DT P

CO USXXAM

PY 1988
 LA Eng
 OS MARPAT 110:58104
 AN CA110(7):58104t
 AB Xn1-X2-W [I; X1 = (blocked) (thionated) amino acid residue; X2 = thionated (blocked) amino acid residue; W = chromogenic or fluorogenic leaving group; n = 0-12] useful in clin. detn. of cysteine proteases, were prepd. Cbz-Arg(Mtr)-OH (Cbz = carbobenzyloxy, Mtr = 4-methoxy-2,3,6-trimethylbenzenesulfonyl) was coupled with 5-aminoisophthalic acid di-Me ester (AIE) via the mixed anhydride method and the product was refluxed 10 h with Lawesson's reagent in C6H6 followed by deprotection with HBr/HOAc to give H-Arg(CS)-AIE.2HBr (CS = thiocarbonyl). The latter was stirred with Cbz-Phe-OTcp (Tcp = trichlorophenyl) in DMF contg. N-methylmorpholine to give Cbz-Phe-Arg(CS)-AIE.HBr. The latter was not hydrolyzed by trypsin but was cleaved by papain with kcat = 5.35.
 IT 111038-22-3P 111070-36-1P 111070-38-3P
 (prepn. of, as intermediate for cysteine protease substrate)
 IT 111070-39-4P
 (prepn. of, as reagent for detn. of cysteine protease)
 IT 111070-40-7P 118406-00-1P 118406-01-2P
 (prepn. of, as reagent for detn. of cysteine proteases)
 L24 ANSWER 10 OF 26 COPYRIGHT 1993 ACS
 AN CA109(11):92639k
 TI Preparation of bisthioamide-7-oxabicycloheptane prostaglandin analogs as antithrombotics
 AU Nakane, Masami; Reid, Joyce
 CS Squibb, E. R., and Sons, Inc.
 LO USA
 SO U.S., 21 pp.
 PI US 4738978 A 19 Apr 1988
 AI US 86-928947 10 Nov 1986
 IC ICM C07D307-00
 ICS C07D405-06; A61K031-34; A61K031-41
 NCL 514382000
 SC 26-3 (Biomolecules and Their Synthetic Analogs)
 SX 1
 DT P
 CO USXXAM
 PY 1988
 LA Eng
 OS MARPAT 109:92639
 AN CA109(11):92639k
 GI

★ I displayed hit
 compounds in this citation
 Look at end of
 search.



AB Title compds. I (A = CH:CH, CH₂CH₂; R = CO₂H, alkoxycarbonyl, tetrazolyl; R₁ = H, alkyl, alkenyl, alkynyl, aryl, arylalkyl, alkoxy, aryloxy, arylsulfonyloxy, etc.; n = 1-5; q = 1-12) their stereoisomers and salts, which are cardiovascular agents, useful, e.g., in the treatment of thrombotic disease (no data), are prepd. tert-Bu [1S-[1.alpha.,2.beta.(5Z),3.beta.,4.alpha.]]-7-[3-[[[1-thioxo-2-[(1-thioxoheptyl)amino]ethyl]amino]methyl]-7-oxabicyclo[2.2.1]hept-2-yl]-5-heptenoate was prepd. in 5 steps from Me [1S-[1.alpha.,2.beta.(5Z),3.beta.,4.alpha.]]-7-[3-(hydroxymethyl)-7-oxabicyclo[2.2.1]hept-2-yl]-5-heptenoate.

IT 115778-41-1P 115778-42-2P
(prepn. of, as antithrombotic)

=> d bib abs hitrn 11-20

L24 ANSWER 11 OF 26 COPYRIGHT 1993 ACS

AN CA108(25):218682u

TI Preparation of vesicles comprising a compound having a hydrophilic peptide radical and use thereof in an assay and kit

AU Wagner, Daniel B.; Piran, Uri

CS Becton, Dickinson and Co.

LO USA

SO U.S., 6 pp.

PI US 4717676 A 5 Jan 1988

AI US 86-835781 3 Mar 1986

IC ICM G01N033-544

NCL 436501000

SC 9-1 (Biochemical Methods)

SX 1, 34

DT P

CO USXXAM

PY 1988

LA Eng

OS MARPAT 108:218682

AN CA108(25):218682u

AB Sacs including a detectable marker and derivatized with a ligand comprise, in part, compd. XYZ (X = hydrophobic radical; Y = hydrophilic peptide; Z = radical including a nonhydrolyzable polar group). Tracer sacs for a digoxin assay were prepd. by dissolving an equimolar mixt. of cholesterol and .beta.-alanylglycylglycyl dioctadecylamide (I) derivatized with a sulfophenyl isothiocyanate and 200 .mu.g I derivatized with digoxin dialdehyde in a 9:1 mixt. of CHCl₃ and MeOH, evapg. to dryness, adding 0.1M sulforhodamine B in water at 60.degree., sonicating, washing with a buffer (310 milliosmolal), and filtering through a 0.4-.mu.m filter.

IT 114515-11-6DP, reaction products with digoxin dialdehyde

114541-93-4P

(prepn. of and tracer sacs contg., for digoxin assay)

L24 ANSWER 12 OF 26 COPYRIGHT 1993 ACS

AN CA106(25):214398s

TI Peptide elastase inhibitors and methods

AU Digenis, George A.; Agha, Bushra J.; Tsuji, Kiyoshi

CS University of Kentucky Research Foundation

LO USA

SO U.S., 24 pp.
PI US 4643991 A 17 Feb 1987
AI US 84-683316 18 Dec 1984
IC ICM A61K037-64
ICS C07K005-08
NCL 514018000
SC 34-3 (Amino Acids, Peptides, and Proteins)
SX 1, 7, 63
DT P
CO USXXAM
PY 1987
LA Eng
AN CA106(25):214398s
AB Z-Ala-Ala-Pro-CH₂-NR₁CO-XR [I; Z = R₂O₂CCH₂CH₂CO (Q); R₂ = alkyl, CF₃CO; X = O, S; R₁ = (cyclo)alkyl, alkenyl, alkynyl, benzyl; R = (un)substituted Ph, CH₂CF₂CF₂CF₃, alkyltetrazolyl, 1-phenyltetrazolyl], having elastase inhibiting activity, are prepd. Peptide coupling of Q-Ala-Ala-OH (R₂ = Me) with H-Pro-CH₂N(CHMe₂)CO₂C₆H₄NO₂-p by a conventional method gave I [Z = Q where R₂ = Me, R = C₆H₄NO₂-p, R₁ = CHMe₂, X = O]. I were tested against trypsin, chymotrypsin, and porcine pancreatic (PP) elastase and were found to have temporary inhibiting effect on PP elastase and no effect on trypsin or chymotrypsin.

IT	92279-32-8P	92279-33-9P	102284-58-2P	102284-60-6P
	102284-61-7P	102306-04-7P	108143-78-8P	108143-82-4P
	108143-85-7P	108143-86-8P	108143-90-4P	108143-94-8P
	108143-98-2P	108155-90-4P	108155-92-6P	108155-98-2P
	108156-01-0P	108156-04-3P	108156-07-6P	108156-10-1P
	108156-13-4P	108156-17-8P	108156-20-3P	108156-25-8P

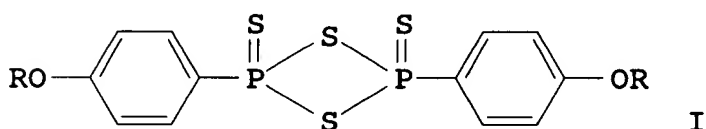
(prepn. of, as elastase inhibitor)

L24 ANSWER 13 OF 26 COPYRIGHT 1993 ACS
AN CA105(3):19458p
TI Inserting amino acid analogs into proteins
AU Rubin, Harvey
LO USA
SO U.S., 6 pp. Cont.-in-part of U.S. Ser. No. 262,303, abandoned.
PI US 4568640 A 4 Feb 1986
AI US 83-476925 21 Mar 1983
PRAI US 81-262303 11 May 1981
IC ICM C12P021-02
NCL 435070000
SC 2-5 (Mammalian Hormones)
SX 6
DT P
CO USXXAM
PY 1986
LA Eng
AN CA105(3):19458p
AB Modified proteins are prepd. by amino acid substitution during translation by means of altered tRNA insertion at a codon to effect incorporation of an amino acid, other than that specified by the mRNA codon, into the translation product. Thus, glutamine acylated glutamic-acid-tRNA [glutamine tRNA] prepd. by mixing glutamic acid-tRNA with glutamine in the presence of tRNA synthetase was incorporated in a translation mixt. contg. endorphin mRNA-enriched polysomes, a 100 .mu.L reticulocyte lysate mixt., and an amino acid

mixt. devoid of glycine, tyrosine, and glutamic acid. The mixt. was incubated for 0 min at 30.degree.. The ACTH/.beta.-lipotropin mol. obtained was treated with clostripain to yield endorphin with glutamic acid-8 substituted by glutamine. The structure was verified by Edman degrdn. Endorphins with phenylalanine 4 and 18 substituted by pNH₂ phenylalanine, with phenylalanines substituted by pCl, with lysine substituted by thiolysine, and with glycine 2 substituted by alanine were similarly prepd. The tRNAs used for substitution may be modified by misacylation or anti-codon alteration.

IT 102790-66-9 102790-67-0 102790-68-1 **102821-96-5**
(formation of, in vitro translation system contg. modified tRNA for)

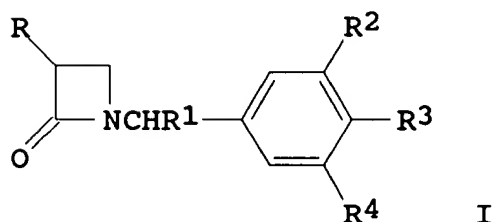
L24 ANSWER 14 OF 26 COPYRIGHT 1993 ACS
AN CA100(23):192077h
TI p-Alkoxyphenylthionophosphine sulfide dimers
AU Belleau, Bernard R.; Franchini, Carlo
CS Bristol-Myers Co.
LO USA
SO U.S., 7 pp.
PI US 4428889 A 31 Jan 1984
AI US 81-263793 14 May 1981
IC C07F009-40; C07C103-52
NCL 260927000R
SC 29-7 (Organometallic and Organometalloidal Compounds)
SX 34
DT P
CO USXXAM
PY 1984
LA Eng
AN CA100(23):192077h
GI



AB Title compds. I (R = C₄-6 alkyl) were prepd. as thiation reagents for peptides. Thus, phenol was o-alkylated with Me(CH₂)₄Br in EtOH contg. NaOEt to give Me(CH₂)₄OPh, which was treated with P₄S₁₀ for 6 h at 150.degree. to give I (R = n-pentyl) (II). Boc-Phe-Met-OMe (Boc = Me₃CO₂C) was thiated by II in THF at room temp. for 24 h to give 80% Boc-NHCH(CH₂Ph)C(S)-Met-OMe.
IT 1071-83-6P 14309-88-7P **90058-16-5P 90058-17-6P**
90058-18-7P 90058-19-8P 90058-20-1P
(prepn. of)

L24 ANSWER 15 OF 26 COPYRIGHT 1993 ACS
AN CA94(9):65461m
TI 4-Unsubstituted azetidinone derivatives
AU Hashimoto, Masashi; Hemmi, Keiji; Kamiya, Takashi; Komori, Tadaaki; Nakaguti, Osamu; Saito, Yoshihisa; Shiokawa, Youichi; Takasugi, Hisahi; Takaya, Takao; Teraji, Tsutomu

CS Fujisawa Pharmaceutical Co., Ltd.
 LO Japan
 SO U.S., 130 pp. Cont.-in-part of U.S. Ser. No. 694,891, abandoned.
 PI US 4207234 10 Jun 1980
 AI US 75-593668 7 Jul 1975
 IC C07D205-08; C07D401-12; C07D403-12; C07D409-12
 NCL 260239000A
 SC 27-5 (Heterocyclic Compounds (One Hetero Atom))
 DT P
 CO USXXAM
 PY 1980
 LA Eng
 AN CA94(9):65461m
 GI



AB Lactacillanic acids and analogs I (R = NH₂, acylamino, benzenesulfonamido; R₁ = CO₂H, pharmaceutically acceptable salt or ester deriv. of CO₂H; R₂ = H, NH₂, NO₂, halo, alkoxy, alkylthio; R₃ = H, OH, alkyl, alkylthio, OCH₂Ph; R₄ = H, Halo, alkoxy, alkylthio), which showed bactericidal activity, were prepd. Thus, 3-aminolactacillanic acid reacted with PhCH₂COCl in water-Me₂CO contg. NaHCO₃ to yield I (R = PhCH₂CONH, R₁ = CO₂H, R₃ = OH, R₂ = R₄ = H).

IT 59510-69-9 59510-71-3 59510-73-5
 59510-75-7

(deacylation of)

IT 59510-70-2P 59510-76-8P

(prepn. and deacylation of)

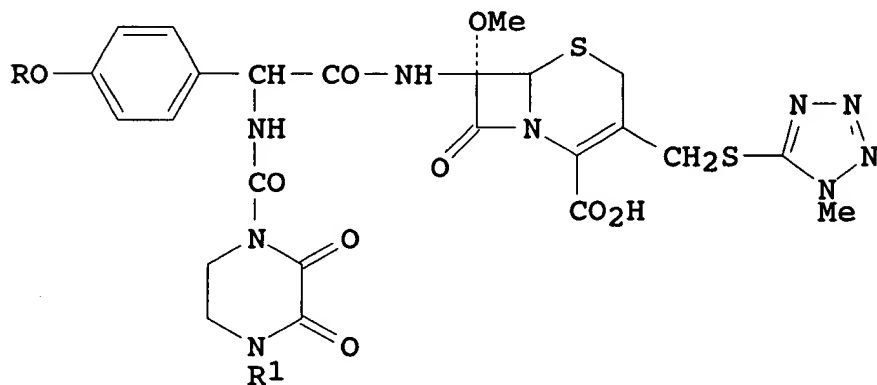
IT	19789-85-6P	30017-02-8P	59508-81-5P	59508-82-6P	59508-84-8P
	59508-85-9P	59508-86-0P	59508-87-1P	59508-88-2P	59508-89-3P
	59508-90-6P	59508-91-7P	59508-94-0P	59508-96-2P	59508-97-3P
	59508-98-4P	59508-99-5P	59509-00-1P	59509-01-2P	59509-02-3P
	59509-03-4P	59509-04-5P	59509-05-6P	59509-06-7P	59509-07-8P
	59509-08-9P	59509-09-0P	59509-10-3P	59509-11-4P	59509-12-5P
	59509-13-6P	59509-14-7P	59509-15-8P	59509-16-9P	59509-17-0P
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(prepn. of)				
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				75261-34-6P

75261-35-7P	75261-38-0P	75261-39-1P	75261-40-4P	75261-41-5P
75269-82-8P	75269-83-9P	75269-85-1P	75270-12-1P	75270-36-9P
75270-43-8P	75270-44-9P	75270-45-0P	75270-46-1P	75270-47-2P
75270-48-3P	75270-49-4P	75270-50-7P	75270-56-3P	
75270-57-4P	75283-26-0P			

(prepn. of)

L24 ANSWER 16 OF 26 COPYRIGHT 1993 ACS
 AN CA93(21):204677f
 TI 7.alpha.-Methoxy substituted cephalosporins
 AU Matsumura, Hiromu; Nagata, Wataru; Narisada, Masayuki; Tsuji, Teruji
 CS Shionogi and Co., Ltd.
 LO Japan
 SO U.S., 6 pp.
 PI US 4211779 8 Jul 1980
 PRAI JP 76-98376 17 Aug 1976
 IC A61K031-545; C07D501-36
 NCL 424246000
 SC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
 DT P
 CO USXXAM
 PY 1980
 LA Eng
 AN CA93(21):204677f
 GI



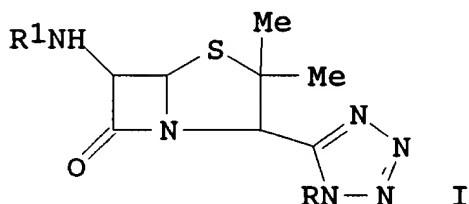
I

AB Cephemcarboxylic acids I (R = H, CONH2, Ac, EtCO, PrCO, CSNH2, methylthiocarbamoyl, CONMe2, CONHCOCCl3, CONHAc, CO2Me, CO2Et, CO2Pr, CO2CHMe2; R1 = Me, Et, Pr, CHMe2, Bu, CHMeEt, CH2CHMe2, CMe3) were prepd. by different methods, and I are useful as bactericides (no data). Benzhydryl 7.alpha.-methoxy-7.beta.-amino-3-[(1-methyl-1H-tetrazol-5-ylthio)methyl]-3-cephem-4-carboxylate was treated with N-(4-ethyl-2,3-dioxo-1-piperazinecarbonyl)-.alpha.-(4-hydroxyphenyl)glycine and ClCOCOC1, and the product was stirred with CF3CO2H in CH2Cl2-PhOMe-C6H6 to give I (R = H, R1 = Et).

IT 64233-55-2P 75500-43-5P 75500-45-7P 75500-46-8P 75500-47-9P
 75500-48-0P 75500-49-1P 75500-50-4P 75500-51-5P 75500-52-6P
 75500-53-7P 75500-54-8P 75500-55-9P 75500-56-0P 75500-57-1P
 75500-58-2P 75500-59-3P 75500-60-6P **75500-61-7P**
 75500-62-8P 75500-63-9P 75500-64-0P 75506-10-4P 75506-11-5P
 75518-67-1P 75518-68-2P

(prepn. of)

L24 ANSWER 17 OF 26 COPYRIGHT 1993 ACS
 AN CA91(5):39467m
 TI Antibacterial 3-(5-tetrazolyl)penam compounds
 AU Barth, Wayne E.
 CS Pfizer Inc.
 LO USA
 SO U.S., 81 pp.
 PI US 4143039 6 Mar 1979
 AI US 73-407097 17 Oct 1973
 IC C07D499-28; C07D499-44
 NCL 260239100
 SC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
 DT P
 CO USXXAM
 PY 1979
 LA Eng
 AN CA91(5):39467m
 GI



AB Title compds. I (R = protective group, R1 = acyl), which exhibited bactericidal activity, were prepd. by different methods. I (R = 4-MeOC6H4CH2, R1 = H) was deprotected by CF3CO2H, and the product was treated with PhCH2COCl to yield I (R = H, R1 = PhCH2CO). Some I were obtained by cyclocondensation of N-substituted 3-penamcarboxamides with tetramethylguanidinium azide.

IT 56852-84-7 56852-85-8 56852-86-9 56852-97-2 69166-89-8
 69166-90-1 69166-91-2 69166-92-3 69166-93-4
 69166-94-5 69179-95-9 70377-03-6

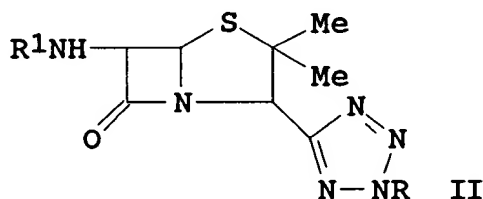
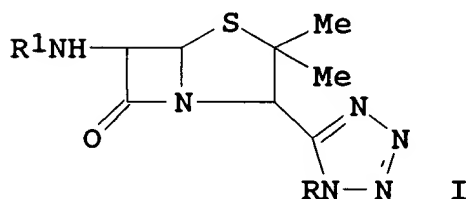
(bactericidal activity of)

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	56852-11-0P	56852-13-2P	56852-14-3P	56852-15-4P	
	56852-16-5P	56852-17-6P	56852-19-8P	56852-21-2P	56852-22-3P
	56852-25-6P	56852-26-7P	56852-29-0P	56852-30-3P	56852-32-5P
	56852-33-6P	56852-34-7P	56852-35-8P	56852-36-9P	56852-37-0P
	56852-38-1P	56852-39-2P	56852-40-5P	56852-41-6P	56852-44-9P
	56852-45-0P	56852-46-1P	56852-47-2P	56852-48-3P	56852-49-4P
	56852-50-7P	56852-51-8P	56852-54-1P	56852-55-2P	56852-56-3P
	56852-57-4P	56852-58-5P	56852-59-6P	56852-63-2P	56852-64-3P
	56852-65-4P	56852-66-5P	56852-67-6P	56852-69-8P	56852-70-1P
	56852-71-2P	56852-72-3P	56852-73-4P	56852-74-5P	56852-76-7P
	56852-78-9P	56852-79-0P	56852-80-3P	56852-81-4P	56852-82-5P
	56852-83-6P	56852-87-0P	56852-88-1P	56852-89-2P	56852-90-5P
	56852-91-6P	56852-92-7P	56852-94-9P	56852-97-2P	56852-99-4P

56853-00-0P	56853-01-1P	56853-02-2P	56853-03-3P	56853-25-9P
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69166-96-7P	69166-99-0P	69167-07-3P	69167-08-4P	69167-11-9P
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69167-27-7P	69167-28-8P	69179-62-0P	69179-71-1P	69179-72-2P
69179-73-3P	69179-74-4P	69179-81-3P	69179-93-7P	69179-98-2P
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69223-26-3P	69223-27-4P	69223-28-5P	69223-30-9P	69223-31-0P
69223-32-1P	69223-33-2P	69223-34-3P	69223-35-4P	69223-36-5P
69223-37-6P	69223-38-7P	69223-39-8P	69223-41-2P	69223-43-4P
69223-44-5P	69223-45-6P	69223-46-7P	69223-48-9P	69223-49-0P
69223-50-3P	69223-52-5P	69223-53-6P	69223-54-7P	69223-56-9P
69223-57-0P	69223-58-1P	69223-59-2P	69223-60-5P	69223-61-6P
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69223-75-2P	69223-76-3P	69223-78-5P	69223-80-9P	69223-84-3P
69223-90-1P	69223-91-2P	69223-92-3P	69223-93-4P	69223-94-5P
69223-95-6P	69223-96-7P	69223-97-8P	69223-98-9P	69223-99-0P
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69224-28-8P	69224-32-4P	69224-34-6P	69224-35-7P	69224-36-8P
69224-37-9P	69224-38-0P	69224-39-1P	69224-40-4P	69224-41-5P
69224-42-6P	69224-43-7P	69224-44-8P	69224-45-9P	69224-46-0P
69224-47-1P	69224-48-2P	69224-49-3P	69224-50-6P	69224-51-7P
69224-52-8P	69224-54-0P	69224-55-1P	69224-56-2P	69224-57-3P
69224-58-4P	69224-59-5P	69224-60-8P	69224-61-9P	69224-62-0P
69224-63-1P	69224-65-3P	69224-66-4P	69224-67-5P	69224-76-6P
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70376-82-8P	70376-87-3P	70376-88-4P	70376-89-5P	
70376-90-8P	70376-95-3P	70376-99-7P	70377-65-0P	70379-35-0P
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(prepn. and bactericidal activity of)				
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56852-86-9P	56854-46-7P	56854-47-8P	56854-50-3P	56854-52-5P
57272-90-9P	57343-08-5P	60099-35-6P	61807-64-5P	61807-77-0P
62306-69-8P	62306-71-2P	69166-41-2P	69166-43-4P	69166-54-7P
69166-57-0P	69166-58-1P	69166-68-3P	69166-72-9P	69166-78-5P
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69223-85-4P	69224-53-9P	69256-21-9P	69256-26-4P	69256-29-7P
69256-56-0P	69815-61-8P	70376-43-1P	70376-44-2P	70376-45-3P
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 (prepn. of)
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 583-39-1 872-35-5 **70379-33-8**
 (S-alkylation by [(chloroacetamido)acetamido]penam deriv.)
 IT **70379-34-9**
 (S-alkylation of thioureas by)

L24 ANSWER 18 OF 26 COPYRIGHT 1993 ACS
 AN CA90(19):152170b
 TI Antibacterial 3-(5-tetrazolyl)penam compounds
 AU Barth, Wayne E.
 CS Pfizer Inc.
 LO USA
 SO U.S., 81 pp.
 PI US 4115385 19 Sep 1978
 AI US 73-407097 17 Oct 1973
 IC C07D499-28
 NCL 260239100
 SC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
 DT P
 CO USXXAM
 PY 1978
 LA Eng
 AN CA90(19):152170b
 GI



AB A series of title compds. I (R = H, trialkylsilyl, alkanoyloxymethyl, 1-alkanoyloxyethyl, 3-phthalidyl; R1 = acyl group of an org. carboxylic acid) were prepd. and exhibited bactericidal activity. Thus, a 3-(N-benzylcarbamoyl)penam deriv. was treated with ClSiMe3 and COCl2 at .apprx.4.degree., tetramethylguanidinium azide was added, the mixt. was agitated at room temp., and the product was desilylated to give I (R = H, R1 = CPh3) (II); II was mixed with 4-MeC6H4SO3H, PhCH2COCl was added, and the mixt. was kept at pH 5.5-6.5 to give I (R = H, R1 = PhCH2CO).

IT 56852-13-2 56852-60-9 56852-97-2 69166-88-7
 69166-89-8 69166-90-1 **69166-91-2** **69166-92-3**
 69166-93-4 69166-94-5
 (bactericidal activity of)

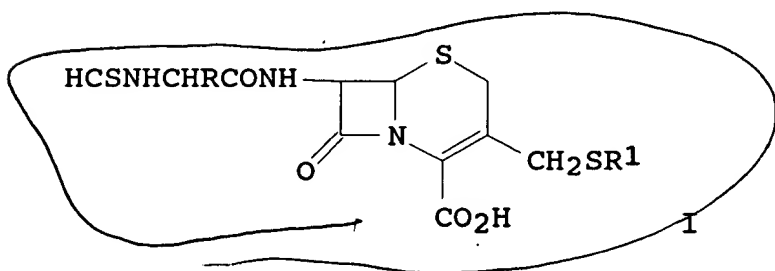
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 56852-11-0P 56852-14-3P 56852-15-4P 56852-16-5P 56852-17-6P
 56852-18-7P 56852-19-8P 56852-21-2P 56852-22-3P 56852-25-6P
 56852-30-3P 56852-32-5P 56852-33-6P 56852-34-7P 56852-35-8P
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56852-57-4P	56852-63-2P	56852-64-3P	56852-65-4P	56852-66-5P
56852-67-6P	56852-69-8P	56852-70-1P	56852-71-2P	56852-72-3P
56852-73-4P	56852-74-5P	56852-75-6P	56852-76-7P	56852-78-9P
56852-79-0P	56852-80-3P	56852-81-4P	56852-82-5P	56852-83-6P
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56854-44-5P	56854-45-6P	56854-48-9P	56968-05-9P	60626-64-4P
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69179-81-3P	69179-91-5P	69179-92-6P	69179-93-7P	69179-95-9P
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69223-18-3P	69223-19-4P	69223-20-7P	69223-23-0P	69223-24-1P
69223-25-2P	69223-26-3P	69223-27-4P	69223-28-5P	69223-29-6P
69223-30-9P	69223-31-0P	69223-32-1P	69223-33-2P	69223-34-3P
69223-35-4P	69223-36-5P	69223-37-6P	69223-38-7P	69223-39-8P
69223-41-2P	69223-42-3P	69223-43-4P	69223-44-5P	69223-45-6P
69223-46-7P	69223-47-8P	69223-48-9P	69223-49-0P	69223-50-3P
69223-51-4P	69223-52-5P	69223-53-6P	69223-54-7P	69223-55-8P
69223-56-9P	69223-57-0P	69223-58-1P	69223-59-2P	69223-60-5P
69223-61-6P	69223-62-7P	69223-63-8P	69223-64-9P	69223-65-0P
69223-67-2P	69223-68-3P	69223-69-4P	69223-70-7P	69223-71-8P
69223-72-9P	69223-73-0P	69223-74-1P	69223-75-2P	69223-77-4P
69223-79-6P	69223-81-0P	69223-83-2P	69223-85-4P	69223-90-1P
69223-91-2P	69223-92-3P	69223-93-4P	69223-94-5P	69223-95-6P
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69224-59-5P	69224-60-8P	69224-61-9P	69224-62-0P	69224-63-1P
69224-64-2P	69224-65-3P	69224-66-4P		
(prepn. and bactericidal activity of)				
IT 56851-82-2P	56851-88-8P	56851-96-8P	56852-13-2P	
56852-41-6P	56852-91-6P	56854-46-7P	56854-47-8P	56854-49-0P
56854-50-3P	56854-52-5P	56937-99-6P	57272-89-6P	57343-08-5P
57403-55-1P	59490-14-1P	60099-35-6P	60099-36-7P	61807-77-0P
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69166-62-7P	69166-65-0P	69166-67-2P	69166-68-3P	69166-70-7P
69166-72-9P	69166-73-0P	69166-75-2P	69166-76-3P	69166-78-5P
69166-79-6P	69166-80-9P	69166-84-3P	69166-85-4P	69166-86-5P
69166-98-9P	69167-04-0P	69167-16-4P	69167-33-5P	69167-36-8P
69167-37-9P	69167-38-0P	69167-39-1P	69167-40-4P	69167-41-5P
69167-42-6P	69167-43-7P	69167-44-8P	69167-46-0P	69167-48-2P
69167-49-3P	69167-50-6P	69167-69-7P	69167-70-0P	69167-71-1P

69179-77-7P	69179-82-4P	69179-84-6P	69179-86-8P	69179-87-9P
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69223-16-1P	69223-21-8P	69223-22-9P	69223-40-1P	69223-66-1P
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69497-77-4P	69815-61-8P	69832-45-7P		

(prepn. of)

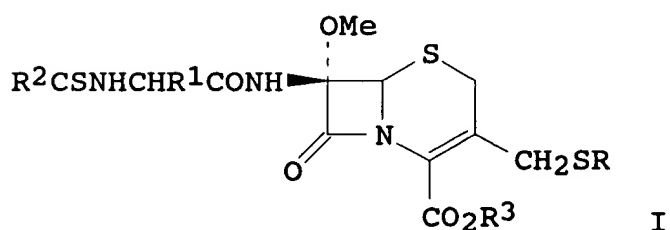
L24 ANSWER 19 OF 26 COPYRIGHT 1993 ACS
 AN CA86(17):121354c
 TI 3-Heterothio derivatives of (.alpha.-thiocarbonylamino) cephalosporins
 AU Breuer, Hermann; Treuner, Uwe D.
 CS Squibb, E. R., and Sons, Inc.
 LO USA
 SO U.S., 8 pp.
 PI US 3996219 7 Dec 1976
 AI US 75-581446 28 May 1975
 IC C07D501-22
 NCL 260243000C
 SC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
 DT P
 CO USXXAM
 PY 1976
 LA Eng
 AN CA86(17):121354c
 GI



AB Cephalosporins I (R = Ph, 2-thienyl, R1 = 1-methyl-5-tetrazolyl; R = Ph, R1 = 5-methyl-1,3,4-thiadiazol-2-yl) were prepd. by treating 7-aminocephalosporanic acid with the heterocyclic thiols, esterifying the cephems, treating the esters with 4-MeOC6H4CH2O2CNHCHRCO2H deblocking, and treating the amines with HCSOEt.
 IT 60891-35-2P 62260-19-9P 62279-87-2P 62279-88-3P
 (prepn. and hydrolysis of)
 IT 36988-22-4P 62260-16-6P 62260-17-7P
 62260-18-8P 62287-60-9P
 (prepn. of)

L24 ANSWER 20 OF 26 COPYRIGHT 1993 ACS
 AN CA86(17):121352a
 TI 3-Heterothio derivatives of (.alpha.-thiocarbonylamino)-7.alpha.-methoxycephalosporins
 AU Breuer, Hermann; Treuner, Uwe D.
 CS Squibb, E. R., and Sons, Inc.

LO USA
 SO U.S., 8 pp.
 PI US 3994889 30 Nov 1976
 AI US 75-581441 28 May 1975
 IC C07D501-24
 NCL 260243000C
 SC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
 DT P
 CO USXXAM
 PY 1976
 LA Eng
 AN CA86(17):121352a
 GI



AB The cephalosporins I (R = 1-methyl-1H-tetrazol-5-yl, R1 = Ph, 2-thienyl, R2 = H; R = 3-methyl-1,2,4-thiadiazol-5-yl, R1 = Ph, 2-thienyl; R2 = H, Me) were prepd. Thus, diphenylmethyl 7-amino-7.alpha.-methoxy-3-[(1-methyl-1H-tetrazol-5-ylthio)methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate was treated with 4-MeOC6H4CH2O2CNHCHPhCO2H followed by F3CCO2H to give 7.beta.-[(aminophenylacetyl)amino]-7.alpha.-methoxy-3-[(1-methyl-1H-tetrazol-5-ylthio)methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid-F3CCO2H, which with Et thioformate gave I (R = 1-methyl-1H-tetrazolyl-5-yl, R1 = Ph, R2 = H).

IT 62202-22-6P 62202-27-1P 62202-30-6P
 (prepn. and reaction with trichloroacetic acid)

IT 62202-25-9P 62202-26-0P 62202-32-8P
 62228-40-4P

(prepn. of)

=> select hit rn 10
 ENTER ANSWER SET L# OR (L24):.
 E1 THROUGH E2 ASSIGNED

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1 115778-41-1/RN
 1 115778-42-2/RN
 L25 2 (115778-41-1/RN OR 115778-42-2/RN)

=> d 1-2

L25 ANSWER 1 OF 2 COPYRIGHT 1993 ACS

RN 115778-42-2 REGISTRY

CN 5-Heptenoic acid, 7-[3-[[[1-thioxo-2-[(1-thioxoheptyl)amino]ethyl]amino]methyl]-7-oxabicyclo[2.2.1]hept-2-yl]-, [1S-[1.alpha.,2.alpha.(Z),3.alpha.,4.alpha.]]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7-Oxabicyclo[2.2.1]heptane, 5-heptenoic acid deriv. (9CI)

MF C23 H38 N2 O3 S2

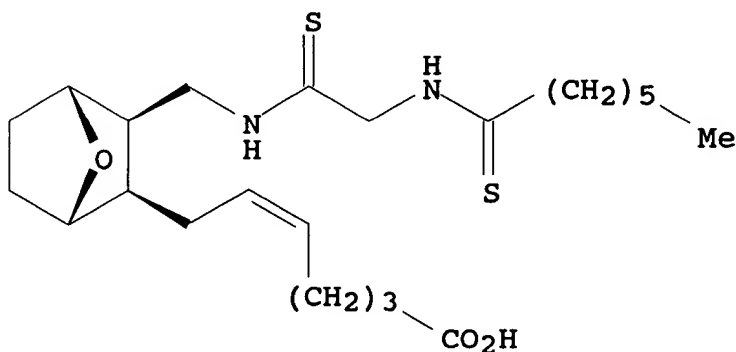
SR CA

LC BEILSTEIN, CA

DES *

Absolute stereochemistry.

Double bond geometry as shown.



2 REFERENCES IN FILE CA (1967 TO DATE)

L25 ANSWER 2 OF 2 COPYRIGHT 1993 ACS

RN 115778-41-1 REGISTRY

CN 5-Heptenoic acid, 7-[3-[[[1-thioxo-2-[(1-thioxoheptyl)amino]ethyl]amino]methyl]-7-oxabicyclo[2.2.1]hept-2-yl]-, 1,1-dimethylethyl ester, [1S-[1.alpha.,2.alpha.(Z),3.alpha.,4.alpha.a.]]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7-Oxabicyclo[2.2.1]heptane, 5-heptenoic acid deriv. (9CI)

MF C27 H46 N2 O3 S2

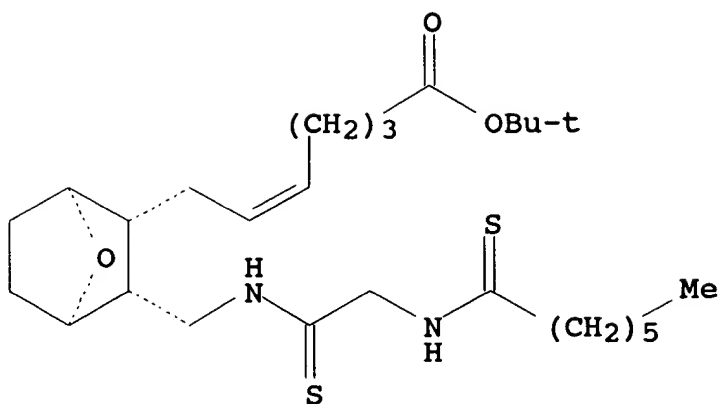
SR CA

LC BEILSTEIN, CA

DES *

Absolute stereochemistry.

Double bond geometry as shown.



1 REFERENCES IN FILE CA (1967 TO DATE)

=> fil reg

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